1.1

a) For FCC, we have

$$\underbrace{8 \times \tfrac{1}{8}}_{\text{corner atoms}} + \underbrace{6 \times \tfrac{1}{2}}_{\text{face atoms}} = \boxed{4 \ \frac{\text{atoms}}{\text{unit cell}}}.$$

b) For BCC, we have

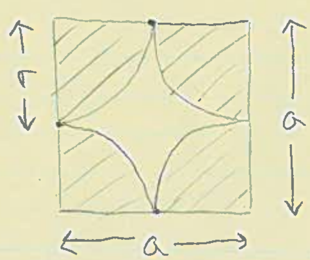
$$\underbrace{8 \times \tfrac{1}{8}}_{\text{corner atoms}} + \underbrace{1}_{\text{center atom}} \boxed{= 2 \ \frac{\text{atoms}}{\text{unit cell}}}$$

c) For diamond we have

$$\underbrace{8 \times \tfrac{1}{8}}_{\text{corner atoms}} + \underbrace{6 \times \tfrac{1}{2}}_{\text{face atoms}} + \underbrace{4}_{\text{center atoms}} \boxed{= 8 \ \frac{\text{atoms}}{\text{unit cell}}}$$

1.2

a) For SC



$$r = \frac{a}{2}$$

$$V_{sphere} = \frac{4}{3}\pi\left(\frac{1}{2}\right)^3 a^3$$

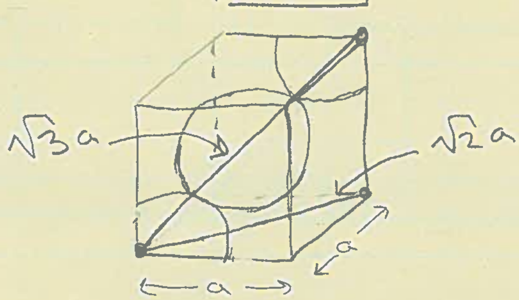
1 atom/unit cell

$$\Rightarrow \text{Packing fraction (PF)} = \frac{\frac{4}{3}\pi\left(\frac{1}{2}\right)^3 a^3}{a^3} = 0.52 \Rightarrow \boxed{52\%}$$

b) For FCC, see in class notes

$$PF = \boxed{74\%}$$

c) For BCC



$$4r = \sqrt{3}a$$

$$r = \frac{\sqrt{3}}{4}a$$

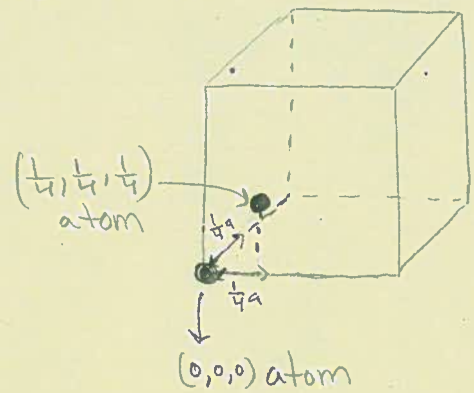
$$V_{sphere} = \frac{4}{3}\pi\left(\frac{\sqrt{3}}{4}\right)^3 a^3$$

BCC has 2 atoms / unit cell

$$V_{TOTAL} = 2 \times \frac{4}{3}\pi\left(\frac{\sqrt{3}}{4}\right)^3 a^3$$

$$\text{so PF} = \frac{2 \times \frac{4}{3}\pi\left(\frac{\sqrt{3}}{4}\right)^3 a^3}{a^3} = 0.68 \Rightarrow \boxed{68\%}$$

d) For diamond.



(0,0,0) and $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ atoms are nearest neighbors, so they touch

the distance between them is $\frac{\sqrt{3}}{4}a$

$$\text{so } 2r = \frac{\sqrt{3}}{4}a$$

$$r = \frac{\sqrt{3}}{8}a$$

$$V_{sphere} = \frac{4}{3}\pi\left(\frac{\sqrt{3}}{8}\right)^3 a^3$$

diamond has 8 atoms / unit cell

$$\text{So PF} = \frac{8 \times \frac{4}{3}\pi\left(\frac{\sqrt{3}}{8}\right)^3 a^3}{a^3} = 0.34 \Rightarrow \boxed{34\%}$$

$\boxed{1.3}$ $a_{Si} = 5.43\ \text{Å} \Longrightarrow$ Si has diamond lattice

a) Distance from one atom to it's nearest neighbor was found in 1.2 d) to be

$$2r = \frac{\sqrt{3}}{4}a \quad \text{center-to-center}$$

For atoms at (0,0,0) and $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$

$$\text{so } 2r = \frac{\sqrt{3}}{4}(5.43\ \text{Å}) = \boxed{2.35\ \text{Å}}$$

b) Number density $= \frac{\text{atoms}}{\text{cm}^3} = \frac{8 \text{ atoms / unit cell}}{(5.43 \times 10^{-8}\ \text{cm})^3}$

$$\boxed{= 5.0 \times 10^{22}\ \frac{\text{atoms}}{\text{cm}^3}}$$

c) mass density = $\frac{g}{cm^3}$

Si atomic weight = 28.06 g/mol

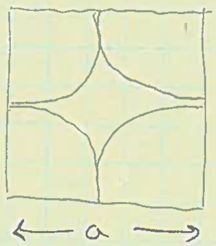
$$MD = \frac{28.06\ g/mol}{6.02 \times 10^{23}\ \frac{atoms}{mol}} \times 5.0 \times 10^{22}\ \frac{atoms}{cm^3}$$

$$\boxed{= 2.33\ g/cm^3}$$

$\boxed{1.7}$

$r = 1.95\ Å$ radius of atom

a) For SC,



$a = 2r \Rightarrow a = 2(1.95\ Å)$

$$\boxed{= 3.9\ Å}$$

b) For FCC, from 1.2b we have $4r = \sqrt{2}a$

$$a = \frac{4r}{\sqrt{2}} = \frac{4(1.95\ Å)}{\sqrt{2}}$$

$$\boxed{= 5.5\ Å}$$

c) For BCC, From 1.2c we have

$$4r = \sqrt{3}a \Rightarrow a = \frac{4}{\sqrt{3}} r = \frac{4}{\sqrt{3}}(1.95 Å)$$

$$\boxed{= 4.5\ Å}$$

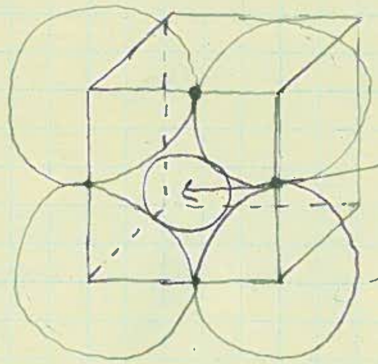
d) For diamond, From 1.2d we have

$$2r = \frac{\sqrt{3}}{4} a \Rightarrow a = \frac{8r}{\sqrt{3}} = \frac{8(1.95\ Å)}{\sqrt{3}}$$

$$\boxed{a = 9.0\ Å}$$

1.8 FCC with element A at corners and element B in the center of each face

$r_A = 1.035\ \text{Å}$



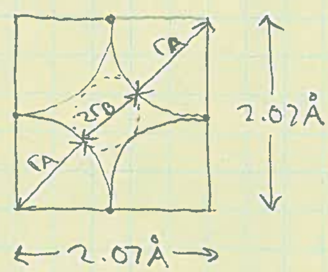
B atom radius?

A atom are touching

a)

Find lattice constant: $2r_A = a = 2(1.035\text{Å}) = 2.07\ \text{Å}$

so we have



side view

the diagonal $= \sqrt{2}\,(2.07\text{Å}) = 2.93\ \text{Å} = 2r_A + 2r_{B_{max}}$

so $r_{B_{max}} = \dfrac{2.93\text{Å} - 2r_A}{2} = \dfrac{2.93\text{Å} - 2(1.035\text{Å})}{2}$

$\boxed{r_{B_{max}} = 0.43\ \text{Å}}$

b) See part a) $\boxed{a = 2.07\ \text{Å}}$

c) volume density for A: $\dfrac{\text{atoms/unit cell}}{\text{volume unit cell}}$

For A-type we have 8 corner atoms $\times \frac{1}{8}$

$= 1$ atom so $VD = \dfrac{1\ \text{atom}}{(2.07\times10^{-8}\text{cm})^3} = \boxed{1.13\times10^{23}\ \frac{\text{atoms}}{\text{cm}^3}}$

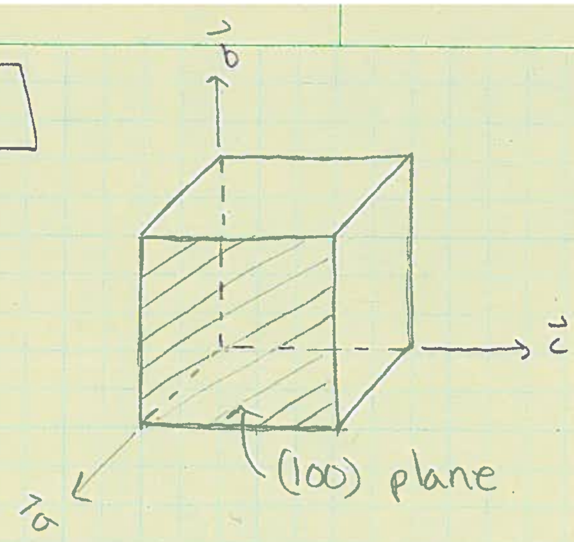
For B-type we have 6 face atoms $\times \frac{1}{2} = 3$ atoms

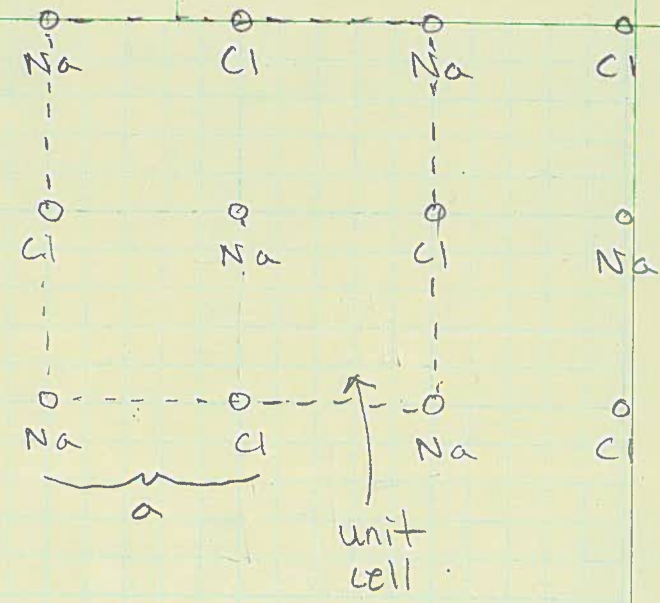
so $VD = \dfrac{3\ \text{atoms}}{(2.07\times10^{-8}\text{cm})^3} = \boxed{3.38\times10^{23}\ \frac{\text{atoms}}{\text{cm}^3}}$

TOPS. 35500

1.11

a)





b) IF $r_{Na} = 1.0\ \text{Å}$ and $r_{Cl} = 1.8\ \text{Å}$

↳ unit cell in (100) plane shown above

$$a = r_{Na} + r_{Cl} = 1.0\ \text{Å} + 1.8\ \text{Å} = \boxed{2.8\ \text{Å}}$$

c) VD for Na atoms and Cl atoms is the same

each 3D unit cell has 4 Na atoms and 4 Cl atoms

$$\text{so VD} = \frac{4 \text{ atoms/unit cell}}{(2a)^3} = \boxed{2.28 \times 10^{22} \frac{\text{atoms}}{\text{cm}^3}}$$

note we used 2a here since the unit cell side is twice that of the lattice constant

d) Mass density = g/cm³

atomic weight Na = 22.99 g/mol

Cl = 35.45 g/mol

there are $2.28 \times 10^{22} \frac{\text{atoms}}{\text{cm}^3}$ for either Na or Cl

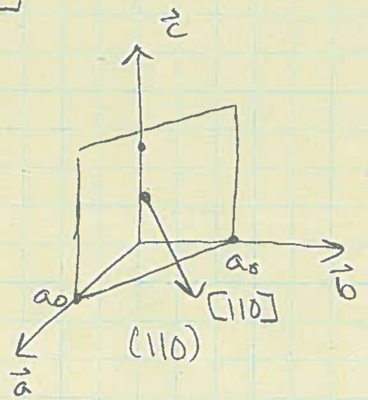
$$\text{so Mass density} = \frac{(22.99 \text{ g/mol} + 35.45 \text{ g/mol})(2.28 \times 10^{22} \frac{\text{ator}}{\text{cm}}}{6.02 \times 10^{23} \text{ atoms/mol}}$$

$$\boxed{= 2.21 \text{ g/cm}^3}$$

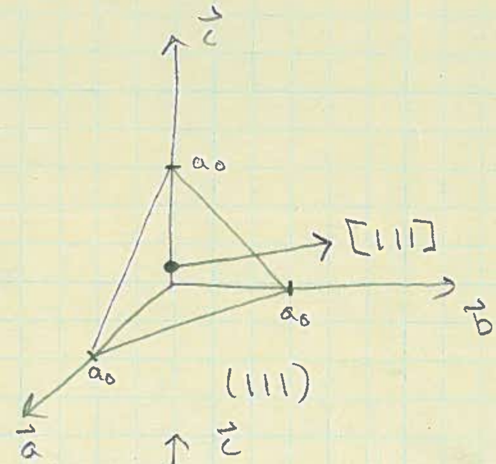
TOPS 35500

1.15

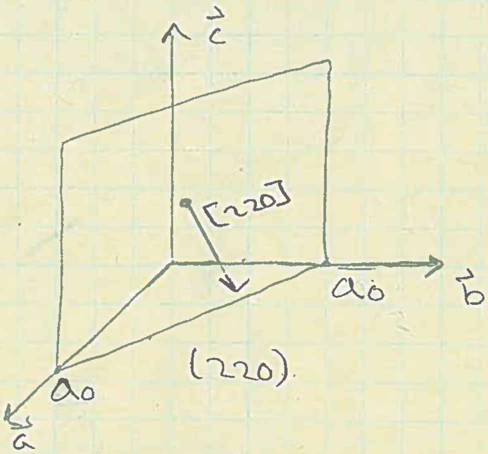
(i)



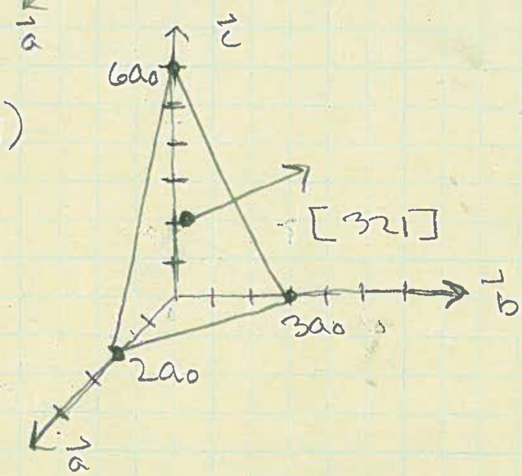
(ii)



(iii)



(iv)



$(220) \Rightarrow \frac{1}{2}, \frac{1}{2}, \infty$

$\Rightarrow$ intercepts $1, 1, \infty$

same as (110) plane

$(321) \Rightarrow \frac{1}{3}\ \frac{1}{2}\ 1$

$\Rightarrow 2, 3, 6$ intercepts

$\boxed{1.16}$

a) intercepts at 1, 3, 1

take reciprocal $\frac{1}{1}, \frac{1}{3}, \frac{1}{1}$

multiply to obtain integers $\Rightarrow$ $\boxed{(313)}$

b) intercepts at 4, 2, 4

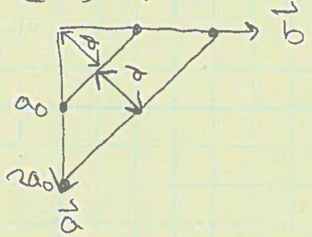
take reciprocal $\frac{1}{4}, \frac{1}{2}, \frac{1}{4}$

multiply to obtain integers $\Rightarrow$ (121)

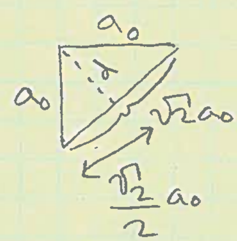
$\boxed{1.18}$ SC structure with $a = 5.28$ Å

a) For (100) planes the next plane is simply one lattice constant away $\boxed{= 5.28 \text{ Å}}$

b) For (110), if we look down the $\vec{c}$ axis we have



Find d:



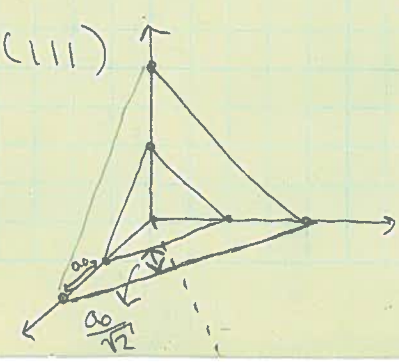
so $a_0^2 = d^2 + \frac{1}{2}a_0^2$

$\frac{1}{2}a_0^2 = d^2$

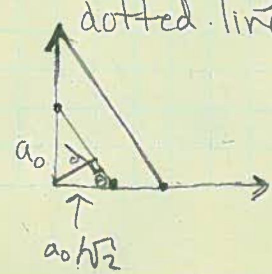
$d = \frac{1}{\sqrt{2}}a_0 = \frac{1}{\sqrt{2}}(5.28 \text{ Å})$

$\boxed{= 3.73 \text{ Å}}$

c) For (111)



side view
slice along
dotted line



$\tan\theta = \frac{a_0}{a_0/\sqrt{2}} = 54.74°$

$d = \frac{a_0}{\sqrt{2}} \sin(54.74°)$ $\boxed{= 3.05 \text{ Å}}$

$\boxed{1.19}$ $a = 4.73\,\text{Å}$

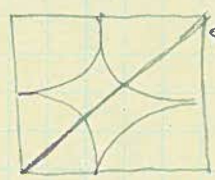
Find surface density

a) SC

i) (100) plane: 1 atom on (100)

$\Longrightarrow SD = \frac{1 \text{ atom}}{(4.73 \times 10^{-8} \text{ cm})^2} = \boxed{4.47 \times 10^{14} \frac{\text{atoms}}{\text{cm}^2}}$

ii) (110) plane

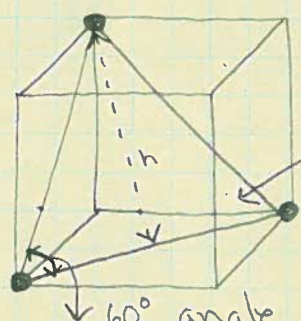


1 atom on (110)

$\Longrightarrow SD = \frac{1 \text{ atom}}{a \cdot \sqrt{2}\, a}$

$= \boxed{3.16 \times 10^{14} \frac{\text{atoms}}{\text{cm}^2}}$

iii)



$\Longrightarrow$ each corner of the triangle intersects $\frac{1}{6}$ of an atom

$\Longrightarrow$ so there are $3 \times \frac{1}{6} = \frac{1}{2}$ atoms on the plane

- now we need the area of the plane

$A = \frac{1}{2}$ base $\cdot$ height

base $= \sqrt{2}\, a$

height: $\left(\frac{\sqrt{2}}{2} a\right)^2 + h^2 = (\sqrt{2}\, a)^2$

$\frac{1}{2} a^2 + h^2 = 2a^2 \Longrightarrow h = \sqrt{\frac{3}{2}}\, a$

so $A = \frac{1}{2} \cancel{\sqrt{2}}\, a \cdot \frac{\sqrt{3}}{\cancel{\sqrt{2}}} a = \frac{\sqrt{3}}{2} a^2$

so $SD = \dfrac{1/2 \text{ atom}}{\frac{\sqrt{3}}{2}(4.73\times10^{-8}\text{cm})^2} = \boxed{2.58\times10^{14}\ \frac{\text{atoms}}{\text{cm}^2}}$

b) BCC

i) (100) has 1 atom

so $SD = \dfrac{1 \text{ atom}}{(4.73\times10^{-8}\text{cm})^2} = \boxed{4.47\times10^{14}\ \frac{\text{atoms}}{\text{cm}^2}}$

ii) (110) has 2 atoms on it and area $\sqrt{2}\,a^2$

so $SD = \dfrac{2 \text{ atoms}}{\sqrt{2}\,a^2} = \boxed{6.32\times10^{14}\ \frac{\text{atoms}}{\text{cm}^2}}$

iii) (111) has $3\times\frac{1}{6} = \frac{1}{2}$ atoms from corners

* the (111) plane does not pass through the center atom

– the area of the (111) plane is again $\frac{\sqrt{3}}{2}a^2$ (see part (a) iii)

so $SD = \dfrac{0.5 \text{ atoms}}{\frac{\sqrt{3}}{2}(4.73\times10^{-8}\text{cm})^2} = \boxed{2.58\times10^{14}\ \frac{\text{atoms}}{\text{cm}^2}}$

c) FCC

i) (100) has 2 atoms on it

so $SD = \dfrac{2 \text{ atoms}}{(4.73\times10^{-8}\text{cm})^2} = \boxed{8.94\times10^{14}\ \frac{\text{atoms}}{\text{cm}^2}}$

ii) (110) has 2 atoms on it

so $SD = \dfrac{2 \text{ atoms}}{\sqrt{2}(4.73\times10^{-8}\text{cm})^2} = \boxed{6.32\times10^{14}\ \frac{\text{atoms}}{\text{cm}^2}}$

iii) (111) has $3\times\frac{1}{6}$ corner atoms = 2 atoms
$3\times\frac{1}{2}$ face atoms

so $SD = \dfrac{2 \text{ atoms}}{\frac{\sqrt{3}}{2}(4.73\times10^{-8}\text{cm})^2} = \boxed{1.03\times10^{15}\ \frac{\text{atoms}}{\text{cm}^2}}$

$\boxed{1.25}$

a) $2\times10^{16}\ cm^{-3}$ of Boron

What is the fraction by weight of Boron?

From 1.3, For Si we have $2.33\ g/cm^3$

For Boron, atomic weight is $10.811\ g/mol$

so the Mass density $= \dfrac{10.811\ g/mol \times 2\times10^{16}\ \frac{atoms}{cm^3}}{6.02\times10^{23}\ atoms/mol}$

$= 3.59\times10^{-7}\ g/cm^3$

so % weight Boron $\simeq \boxed{100\% \times \dfrac{3.59\times10^{-7}\ g/cm^3}{2.33\ g/cm^3} = 1.54\times10^{-5}\ \%}$

or $\boxed{1.54\times10^{-7}\ \text{fraction}}$

b) For phosphorous $1\times10^{18}\ atoms/cm^3$

atomic weight $= 30.97\ g/mol$

the mass density is $= \dfrac{30.97\ g/mol \times 1\times10^{18}\ \frac{atoms}{cm^3}}{6.02\times10^{23}\ atoms/mol}$

$= 5.14\times10^{-5}\ g/cm^3$

So % weight Phosphors

$\simeq 100\% \times \dfrac{5.14\times10^{-5}\ g/cm^3}{2.33\ g/cm^3} = 0.00221$

or $\boxed{2.21\times10^{-5}\ \text{fraction}}$

neglecting B and P in the denominator since they are small